

# Poly[bis(*N,N*-dimethylformamide- $\kappa$ O)-( $\mu_4$ -naphthalene-1,5-disulfonato)-magnesium(II)]

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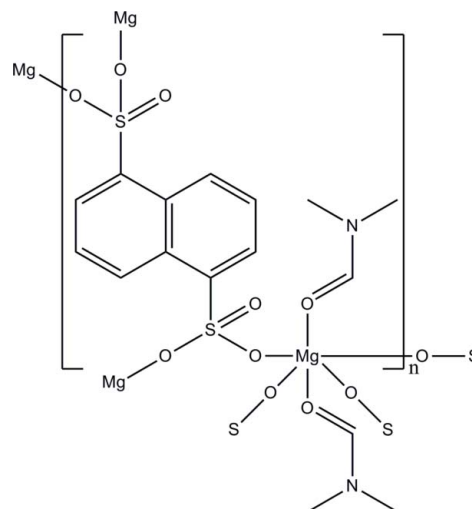
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Key indicators: single-crystal synchrotron study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å; disorder in main residue;  $R$  factor = 0.032;  $wR$  factor = 0.087; data-to-parameter ratio = 8.9.

The structure of the title compound,  $[\text{Mg}(\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)(\text{C}_3\text{H}_7\text{NO})_2]_n$ , consists of  $\text{MgO}_6$  octahedra ( $\bar{1}$  symmetry) connected to naphthalene-1,5-disulfonate ligands ( $\bar{1}$  symmetry) in the equatorial plane, forming a two-dimensional network propagating parallel to (010). The coordination sphere of the Mg atom is completed by the O atoms of two *N,N*-dimethylformamide (DMF) molecules in the axial positions. The title compound represents the first time the naphthalene-1,5-disulfonate anion is bound directly to a  $\text{Mg}^{2+}$  atom. Disorder over two positions was found in the DMF molecule in a 0.518 (8):0.482 (8) ratio.

## Related literature

For background to metal-organic coordination polymers (CPs) and frameworks (MOFs), see: Cheetham *et al.* (2006); Kitagawa *et al.* (2004); Rosseinsky (2004); Rowsell & Yaghi (2004). For structures in which  $\text{Mg}^{2+}$  is not directly linked to naphthalenedisulfonate ligands but is surrounded by water molecules, see: Cody & Hazel (1977); Morris *et al.* (2003); Shakeri & Haussühl (1992).



## Experimental

### Crystal data

$[\text{Mg}(\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)(\text{C}_3\text{H}_7\text{NO})_2]$   
 $M_r = 456.79$   
 Triclinic,  $P\bar{1}$   
 $a = 5.1328$  (2) Å  
 $b = 9.3890$  (4) Å  
 $c = 10.4029$  (4) Å  
 $\alpha = 85.158$  (1)°  
 $\beta = 75.638$  (1)°

$\gamma = 79.501$  (1)°  
 $V = 477.13$  (3) Å<sup>3</sup>  
 $Z = 1$   
 Synchrotron radiation  
 $\lambda = 0.41328$  Å  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.09 \times 0.03 \times 0.01$  mm

### Data collection

Bruker APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2008)  
 $T_{\min} = 0.993$ ,  $T_{\max} = 0.999$

8811 measured reflections  
 1961 independent reflections  
 1721 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.054$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.087$   
 $S = 1.04$   
 1961 reflections  
 221 parameters

6 restraints  
 Only H-atom coordinates refined  
 $\Delta\rho_{\max} = 0.61$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.51$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Mg1—O1	2.0193 (11)	Mg1—O4	2.1562 (11)
Mg1—O2 <sup>i</sup>	2.0429 (11)		

Symmetry code: (i)  $x + 1, y, z$ .

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT-Plus (Bruker, 2007); data reduction: SAINT-Plus; program(s) used to solve structure: SIR2004 (Burla *et al.*, 2005); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: CrystalMaker (CrystalMaker, 2009); software used to prepare material for publication: enCIFer (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2328).

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**supplementary materials**

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## Poly[bis(*N,N*-dimethylformamide- $\kappa$ O)( $\mu_4$ -naphthalene-1,5-disulfonato)magnesium(II)]

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### Comment

Interest in metal organic coordination polymers (CPs) and frameworks (MOFs) arises due to the potential applications including size/shape catalysis and gas storage/separation (Cheetham *et al.*, 2006; Kitagawa *et al.*, 2004; Rosseinsky, 2004; Rowsell & Yaghi, 2004). This is owing to the fact that these materials have similar properties to zeolites with the added possibility of structural design. Three factors need to be considered during the synthesis of CPs and MOFs; the coordination sphere of the metal center, the size, shape and functionality of the organic linker and the synthetic conditions.

Previous studies have looked at the interaction between a variety of metal atoms and 1,5-naphthalenedisulfonic acid. A search of the literature results in examples of direct bonding between this ligand and every alkali and alkali earth metal except  $\text{Mg}^{2+}$ . Due to periodic trends we suspected that  $\text{Mg}^{2+}$  and naphthalene-1,5-disulfonate should have a direct bonding interaction, which indicates a change in synthetic conditions compared to the previous studies was needed. The previous efforts used water as the solvent resulting in structures where the  $\text{Mg}^{2+}$  atoms are bound solely to water molecules and interacted with 1,5-naphthalenedisulfonic acid through hydrogen bonds (Cody & Hazel, 1977; Morris *et al.*, 2003; Shakeri & Haussühl, 1992). In our study we used *N,N*-dimethylformamide (DMF) as the solvent with the thought that DMF is a large solvent molecule and is unlikely to complete for the coordination sphere of the  $\text{Mg}^{2+}$  atom.

The title compound consists of  $\text{MgO}_6$  octahedra linked by 1,5-naphthalenedisulfonate ligands to form a two-dimensional network parallel to (010). The  $\text{Mg}^{2+}$  atom is bound to four O atoms from four separate naphthalene-1,5-disulfonate ligands in the equatorial plane and two O atoms from two symmetry equivalent *N,N*-dimethylformamide molecules in the axial positions (Figure 1). The average equatorial Mg—O bond length is 2.031 Å whereas the axial bond length is slightly longer at 2.156 Å (Table 1). The individual  $\text{MgO}_6$  octahedra are connected by the naphthalene-1,5-disulfonate linkers in a bridging bidentate fashion to form chains along the [100] direction, which are further connected by the linker molecules to form an overall 2-dimensional structure (Figure 2).

### Experimental

All of the starting materials are available commercially and were used without any further purification. Magnesium nitrate hexahydrate ( $\text{Mg}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ , 1.3 grams), 1,5-naphthalenedisulfonic acid tetrahydrate ( $\text{C}_{10}\text{H}_8\text{S}_2\text{O}_6 \cdot 4\text{H}_2\text{O}$ , 1.87 grams) and ammonium fluoride ( $\text{NH}_4\text{F}$ , 0.021 grams) were dissolved in 15 grams of *N,N*-dimethylformamide (DMF). The solution was prepared in a 23 mL Teflon lined Parr bomb and stirred for three hours to achieve homogeneity. The resulting solution was heated statically at 373 K for three days. Colorless needle shaped crystals were recovered and were washed with ethanol.

## Refinement

Disorder was found in the bound *N,N*-dimethylformamide molecules with the major component occupied 51.8 (8)% and the minor 48.2 (8)%, of which only the O atom does not have a second position. The disordered atoms were refined anisotropically without constraints. All of the hydrogen atoms were located in the Fourier difference map and their positions were allowed to refine independent of the C atoms with  $U_{\text{iso}}(\text{H})=1.5U_{\text{eq}}(\text{C})$  for the methyl groups and  $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C})$  for all others. The highest peak ( $\sim 0.6 \text{ e}^- \text{ \AA}^{-3}$ ) can be found within 0.89 Å of C2 and the deepest hole ( $\sim -0.5 \text{ e}^- \text{ \AA}^{-3}$ ) within 0.73 Å of S1. The near equal values of the highest peak and deepest hole indicate that there is not any remaining unmodelled electron density. The crystal remained stable throughout the low temperature data collection.

## Figures



Fig. 1. Polyhedral representation of a layer of the title compound. The DMF disorder and the H atoms were omitted for clarity. Color codes: blue octahedra Mg, red spheres O, light blue spheres N, and black lines C.

## Poly[bis(*N,N*-dimethylformamide- $\kappa$ O)( $\mu_4$ - naphthalene-1,5-disulfonato)magnesium(II)]

### Crystal data

[Mg(C<sub>10</sub>H<sub>6</sub>O<sub>6</sub>S<sub>2</sub>)(C<sub>3</sub>H<sub>7</sub>NO)<sub>2</sub>]

$M_r = 456.79$

Triclinic, *P* $\bar{1}$

Hall symbol: -P 1

$a = 5.1328 (2) \text{ \AA}$

$b = 9.3890 (4) \text{ \AA}$

$c = 10.4029 (4) \text{ \AA}$

$\alpha = 85.158 (1)^\circ$

$\beta = 75.638 (1)^\circ$

$\gamma = 79.501 (1)^\circ$

$V = 477.13 (3) \text{ \AA}^3$

$Z = 1$

$F(000) = 238$

$D_x = 1.590 \text{ Mg m}^{-3}$

Synchrotron radiation,  $\lambda = 0.41328 \text{ \AA}$

Cell parameters from 4827 reflections

$\theta = 2.4\text{--}17.1^\circ$

$\mu = 0.08 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Needle, colorless

$0.09 \times 0.03 \times 0.01 \text{ mm}$

### Data collection

Bruker APEXII CCD  
diffractometer

Radiation source: APS Sector 15

graphite

phi scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2008)

$T_{\text{min}} = 0.993$ ,  $T_{\text{max}} = 0.999$

8811 measured reflections

1961 independent reflections

1721 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.054$

$\theta_{\text{max}} = 15.0^\circ$ ,  $\theta_{\text{min}} = 1.3^\circ$

$h = -6 \rightarrow 6$

$k = -11 \rightarrow 11$

$l = -12 \rightarrow 12$

Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.032$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.087$	Only H-atom coordinates refined
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.2091P]$
1961 reflections	where $P = (F_o^2 + 2F_c^2)/3$
221 parameters	$(\Delta/\sigma)_{\max} < 0.001$
6 restraints	$\Delta\rho_{\max} = 0.61 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.51 \text{ e } \text{\AA}^{-3}$

Special details

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
S1	0.07457 (7)	0.11525 (4)	0.80723 (4)	0.00723 (15)	
Mg1	0.5000	0.0000	1.0000	0.00731 (19)	
O1	0.2916 (2)	0.11924 (12)	0.87562 (11)	0.0100 (3)	
O2	-0.1359 (2)	0.04071 (13)	0.88296 (11)	0.0117 (3)	
O3	-0.0320 (2)	0.25885 (12)	0.76873 (12)	0.0123 (3)	
O4	0.5528 (2)	-0.18505 (12)	0.88102 (12)	0.0115 (3)	
C1	0.4500 (3)	0.04297 (17)	0.56082 (16)	0.0084 (3)	
C2	0.2241 (3)	0.00625 (17)	0.65774 (15)	0.0088 (3)	
C3	0.1051 (3)	-0.10819 (18)	0.63682 (17)	0.0113 (3)	
H3	-0.048 (4)	-0.127 (2)	0.698 (2)	0.014*	
C4	0.4211 (3)	-0.16097 (18)	0.42018 (17)	0.0103 (3)	
H4	0.474 (4)	-0.216 (2)	0.343 (2)	0.012*	
C5	0.2054 (4)	-0.19167 (19)	0.51598 (17)	0.0135 (4)	
H5	0.112 (4)	-0.269 (2)	0.503 (2)	0.016*	
C6	0.3941 (13)	-0.2695 (7)	0.8776 (6)	0.0152 (12)	0.518 (8)
H6	0.213 (9)	-0.258 (4)	0.935 (4)	0.018*	0.518 (8)
N1	0.4566 (15)	-0.3857 (7)	0.7960 (6)	0.0128 (13)	0.518 (8)
C7	0.2600 (9)	-0.4804 (5)	0.7982 (5)	0.0269 (13)	0.518 (8)

## supplementary materials

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H7A	0.355 (14)	-0.580 (7)	0.827 (7)	0.040*	0.518 (8)
H7B	0.089 (11)	-0.435 (6)	0.866 (5)	0.040*	0.518 (8)
H7C	0.224 (10)	-0.489 (6)	0.713 (6)	0.040*	0.518 (8)
C8	0.7147 (16)	-0.4185 (7)	0.6958 (6)	0.0182 (13)	0.518 (8)
H8A	0.809 (13)	-0.505 (9)	0.686 (7)	0.027*	0.518 (8)
H8B	0.683 (11)	-0.383 (6)	0.620 (5)	0.027*	0.518 (8)
H8C	0.839 (10)	-0.384 (5)	0.721 (5)	0.027*	0.518 (8)
C6'	0.4544 (12)	-0.2955 (6)	0.9149 (6)	0.0098 (11)	0.482 (8)
H6'	0.362 (9)	-0.313 (5)	1.007 (5)	0.012*	0.482 (8)
N1'	0.4704 (16)	-0.4086 (8)	0.8350 (7)	0.0108 (13)	0.482 (8)
C7'	0.3529 (8)	-0.5363 (4)	0.8827 (4)	0.0154 (13)	0.482 (8)
H7A'	0.228 (11)	-0.544 (8)	0.839 (6)	0.023*	0.482 (8)
H7B'	0.500 (10)	-0.625 (5)	0.860 (5)	0.023*	0.482 (8)
H7C'	0.279 (9)	-0.520 (5)	0.977 (5)	0.023*	0.482 (8)
C8'	0.6042 (17)	-0.4110 (8)	0.6929 (6)	0.0157 (14)	0.482 (8)
H8A'	0.751 (13)	-0.511 (9)	0.678 (7)	0.024*	0.482 (8)
H8B'	0.674 (10)	-0.320 (6)	0.674 (5)	0.024*	0.482 (8)
H8C'	0.469 (11)	-0.418 (5)	0.651 (5)	0.024*	0.482 (8)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0075 (2)	0.0079 (2)	0.0062 (2)	-0.00348 (15)	-0.00026 (15)	0.00097 (15)
Mg1	0.0080 (4)	0.0073 (4)	0.0069 (4)	-0.0044 (3)	-0.0006 (3)	0.0014 (3)
O1	0.0109 (5)	0.0108 (6)	0.0091 (6)	-0.0057 (4)	-0.0027 (4)	0.0039 (5)
O2	0.0097 (5)	0.0156 (6)	0.0103 (6)	-0.0080 (5)	0.0006 (4)	0.0010 (5)
O3	0.0140 (6)	0.0089 (6)	0.0134 (6)	-0.0014 (5)	-0.0038 (5)	0.0028 (5)
O4	0.0138 (6)	0.0098 (6)	0.0116 (6)	-0.0058 (5)	-0.0016 (5)	0.0002 (5)
C1	0.0093 (7)	0.0077 (8)	0.0085 (8)	-0.0017 (6)	-0.0031 (6)	0.0018 (6)
C2	0.0099 (7)	0.0090 (8)	0.0072 (8)	-0.0012 (6)	-0.0022 (6)	0.0009 (6)
C3	0.0116 (8)	0.0126 (8)	0.0098 (8)	-0.0062 (6)	-0.0005 (6)	0.0025 (6)
C4	0.0138 (8)	0.0093 (8)	0.0083 (8)	-0.0051 (6)	-0.0013 (6)	-0.0007 (6)
C5	0.0173 (8)	0.0120 (8)	0.0134 (8)	-0.0104 (7)	-0.0019 (7)	-0.0004 (7)
C6	0.016 (3)	0.020 (3)	0.012 (3)	-0.0077 (19)	-0.0046 (19)	-0.001 (2)
N1	0.020 (2)	0.010 (2)	0.011 (3)	-0.0105 (18)	-0.004 (2)	0.002 (2)
C7	0.032 (2)	0.022 (2)	0.031 (3)	-0.0188 (19)	-0.0045 (19)	-0.0054 (19)
C8	0.020 (3)	0.015 (3)	0.017 (2)	-0.001 (3)	-0.002 (3)	-0.0009 (16)
C6'	0.010 (2)	0.011 (2)	0.010 (3)	-0.0038 (18)	-0.0023 (18)	-0.004 (2)
N1'	0.012 (2)	0.008 (2)	0.010 (3)	-0.0034 (17)	0.000 (2)	0.002 (2)
C7'	0.0156 (19)	0.008 (2)	0.022 (3)	-0.0054 (14)	-0.0012 (16)	-0.0012 (16)
C8'	0.018 (3)	0.016 (2)	0.014 (3)	-0.004 (3)	-0.003 (3)	-0.0018 (16)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

S1—O3	1.4234 (12)	C5—H5	0.98 (2)
S1—O2	1.4276 (12)	C6—N1	1.381 (8)
S1—O1	1.4701 (11)	C6—H6	0.97 (4)
S1—C2	1.8560 (16)	N1—C7	1.456 (7)
Mg1—O1	2.0193 (11)	N1—C8	1.469 (9)

Mg1—O1 <sup>i</sup>	2.0193 (11)	C7—H7A	1.03 (7)
Mg1—O2 <sup>ii</sup>	2.0429 (11)	C7—H7B	1.03 (6)
Mg1—O2 <sup>iii</sup>	2.0429 (11)	C7—H7C	0.97 (6)
Mg1—O4 <sup>i</sup>	2.1562 (11)	C8—H8A	0.87 (9)
Mg1—O4	2.1562 (11)	C8—H8B	0.87 (5)
O2—Mg1 <sup>iv</sup>	2.0429 (11)	C8—H8C	0.87 (5)
O4—C6'	1.223 (6)	C6'—N1'	1.382 (8)
O4—C6	1.244 (6)	C6'—H6'	0.97 (5)
C1—C2	1.409 (2)	N1'—C7'	1.436 (7)
C1—C4 <sup>v</sup>	1.440 (2)	N1'—C8'	1.468 (8)
C1—C1 <sup>v</sup>	1.488 (3)	C7'—H7A'	0.89 (6)
C2—C3	1.386 (2)	C7'—H7B'	1.02 (5)
C3—C5	1.469 (2)	C7'—H7C'	0.97 (5)
C3—H3	0.92 (2)	C8'—H8A'	1.09 (9)
C4—C5	1.350 (2)	C8'—H8B'	0.98 (5)
C4—C1 <sup>v</sup>	1.440 (2)	C8'—H8C'	0.92 (5)
C4—H4	0.95 (2)		
O3—S1—O2	111.65 (7)	C3—C5—H5	119.7 (12)
O3—S1—O1	109.59 (7)	O4—C6—N1	124.7 (6)
O2—S1—O1	113.33 (7)	O4—C6—H6	120 (2)
O3—S1—C2	109.78 (7)	N1—C6—H6	115 (2)
O2—S1—C2	104.07 (7)	O4—C6—H6'	94.7 (18)
O1—S1—C2	108.22 (7)	N1—C6—H6'	111.8 (18)
O1—Mg1—O1 <sup>i</sup>	180.00 (4)	H6—C6—H6'	61 (3)
O1—Mg1—O2 <sup>ii</sup>	91.70 (5)	C6—N1—C7	121.5 (6)
O1 <sup>i</sup> —Mg1—O2 <sup>ii</sup>	88.30 (5)	C6—N1—C8	123.5 (6)
O1—Mg1—O2 <sup>iii</sup>	88.30 (5)	C7—N1—C8	114.9 (6)
O1 <sup>i</sup> —Mg1—O2 <sup>iii</sup>	91.70 (5)	N1—C7—H7A	103 (4)
O2 <sup>ii</sup> —Mg1—O2 <sup>iii</sup>	180.0	N1—C7—H7B	104 (3)
O1—Mg1—O4 <sup>i</sup>	90.98 (5)	H7A—C7—H7B	115 (5)
O1 <sup>i</sup> —Mg1—O4 <sup>i</sup>	89.02 (5)	N1—C7—H7C	114 (3)
O2 <sup>ii</sup> —Mg1—O4 <sup>i</sup>	93.38 (5)	H7A—C7—H7C	108 (5)
O2 <sup>iii</sup> —Mg1—O4 <sup>i</sup>	86.62 (4)	H7B—C7—H7C	112 (4)
O1—Mg1—O4	89.02 (5)	N1—C8—H8A	123 (5)
O1 <sup>i</sup> —Mg1—O4	90.98 (5)	N1—C8—H8B	107 (4)
O2 <sup>ii</sup> —Mg1—O4	86.62 (4)	H8A—C8—H8B	110 (6)
O2 <sup>iii</sup> —Mg1—O4	93.38 (5)	N1—C8—H8C	108 (3)
O4 <sup>i</sup> —Mg1—O4	180.0	H8A—C8—H8C	94 (5)
S1—O1—Mg1	141.82 (7)	H8B—C8—H8C	115 (5)
S1—O2—Mg1 <sup>iv</sup>	161.80 (8)	N1'—C6'—H6'	113 (2)
C6'—O4—Mg1	126.6 (3)	C6'—N1'—C7'	123.1 (5)
C6—O4—Mg1	130.9 (3)	C6'—N1'—C8'	124.2 (6)
C2—C1—C4 <sup>v</sup>	120.44 (15)	C7'—N1'—C8'	112.7 (6)
C2—C1—C1 <sup>v</sup>	118.31 (17)	N1'—C7'—H7A'	109 (5)



## supplementary materials

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C4 <sup>v</sup> —C1—C1 <sup>v</sup>	121.26 (18)	N1'—C7'—H7B'	109 (3)
C3—C2—C1	119.08 (15)	H7A'—C7'—H7B'	106 (5)
C3—C2—S1	120.03 (12)	N1'—C7'—H7C'	103 (3)
C1—C2—S1	120.80 (12)	H7A'—C7'—H7C'	114 (5)
C2—C3—C5	122.01 (15)	H7B'—C7'—H7C'	116 (4)
C2—C3—H3	117.9 (12)	N1'—C8'—H8A'	107 (4)
C5—C3—H3	119.9 (12)	N1'—C8'—H8B'	104 (3)
C5—C4—C1 <sup>v</sup>	118.10 (15)	H8A'—C8'—H8B'	118 (5)
C5—C4—H4	118.1 (12)	N1'—C8'—H8C'	105 (3)
C1 <sup>v</sup> —C4—H4	123.7 (12)	H8A'—C8'—H8C'	107 (4)
C4—C5—C3	121.24 (15)	H8B'—C8'—H8C'	115 (4)
C4—C5—H5	119.0 (12)		

Symmetry codes: (i)  $-x+1, -y, -z+2$ ; (ii)  $x+1, y, z$ ; (iii)  $-x, -y, -z+2$ ; (iv)  $x-1, y, z$ ; (v)  $-x+1, -y, -z+1$ .

Fig. 1

